

Abstract (250 Words max)

New modeling approaches to study DNA damage by the direct and indirect effects of ionizing radiation

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DNA is damaged both by the direct and indirect effects of radiation. In the direct effect, the DNA itself is ionized, whereas the indirect effect involves the radiolysis of the water molecules surrounding the DNA and the subsequent reaction of the DNA with radical products. While this problem has been studied for many years, many unknowns still exist. To study this problem, we have developed the computer code RITRACKS [1], which simulates the radiation track structure for heavy ions and electrons, calculating all energy deposition events and the coordinates of all species produced by the water radiolysis. In this work, we plan to simulate DNA damage by using the crystal structure of a nucleosome and calculations performed by RITRACKS. The energy deposition events are used to calculate the dose deposited in nanovolumes [2] and therefore can be used to simulate the direct effect of the radiation. Using the positions of the radiolytic species with a radiation chemistry code [3] it will be possible to simulate DNA damage by indirect effect. The simulation results can be compared with results from previous calculations such as the frequencies of simple and complex strand breaks [4] and with newer experimental data using surrogate markers of DNA double-strand breaks such as γ -H2AX foci [5]. References: [1] New J. Phys. 10, 125020 (2008); [2] Radiat. Prot. Dosim. 143, 156-161 (2011); [3] Radiat. Env. Biophys. 3, 389-403 (2011). [4] Int. J. Radiat. Biol. 71, 467 (1997); [5] Radiat. Res. 169, 437-483 (2008).